Spin-Spin Interaction In Artificial Molecules With In-Plane Magnetic Field

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Abstract

We investigate theoretically the spin-spin interaction of two-electrons in vertically coupled QDs as a function of the angle between magnetic field and growth axis. Our numerical approach is based on a real-space description of single-particle states in realistic samples and exact diagonalization of carrier-carrier Coulomb interaction. In particular, the effect of the in-plane field component on tunneling and, therefore, spin-spin interaction will be discussed; the singlet-triplet phase diagram as a function of the field strength and direction is drawn.

Key words: quantum dots, semiconductor, quantum phase, magnetic field, spin-spin interaction, exchange energy
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1 Introduction

Coupled quantum dots, also called Artificial Molecules (AM), extend to the molecular realm the similarity between quantum dots (QDs) and artificial atoms [1,2]. Inter-dot tunneling introduces an energy scale which may be comparable to other energy scales in the system, namely, single-particle confinement energies, carrier-carrier interaction, and magnetic energy.

In AMs carriers sitting on either dot are not only electrostatically coupled, but also have their spin interlaced when tunneling is allowed [3]. This is sketched in

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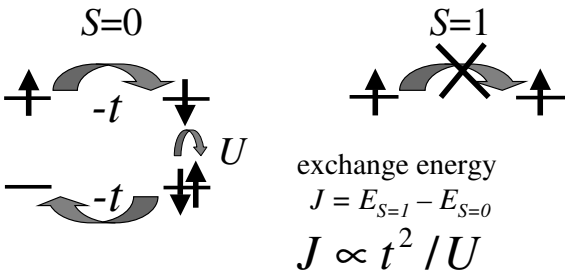

Fig. 1. Sketch of the energy contributions to the tunneling-induced spin-spin interaction.

Fig. 1. For two electrons in a singlet state it is possible to tunnel into the same dot. By doing so, they gain the tunneling energy t; this may compensate for the loss in the Coulomb energy U. This process is forbidden for two electrons in the triplet state by Pauli blocking. Different spin orderings, therefore, are associated to an exchange energy $J \propto t^2/U$. While in real molecules J is fixed by the bond length, in AMs it is possible to tune all energy scales by sample engineering and external fields.

One convenient way to control inter-dot tunneling, and, hence, effective spin-spin interaction, is by applying a magnetic field with a finite component perpendicular to the tunneling direction. This is particularly important in vertically coupled QDs, where otherwise tunneling in a given sample is fixed by sample parameters; this extends the use of a vertical field, $B_\perp$, to drive the system from a low correlation (low field) regime to a high correlation (high field) one [4]. In addition to the vertical component of the field, therefore, a magnetic field in the plane of the QD, $B_\parallel$, can be used to fully control the spin-spin interaction and, therefore, the spin character of the ground state of few-electron systems.

In this paper we discuss theoretically the two-electron phase diagram, with particular respect to the spin ordering, in vertically coupled QDs in the ($B_\perp$,$B_\parallel$) plane. Our numerical approach is based on a real-space description of single-particle states which fully includes the complexity of typical samples, i.e., layer width, finite band-offsets etc. We include carrier-carrier Coulomb interaction, represented in a Slater determinant basis, by exact diagonalization methods.

2 Single particle states

In the symmetric coupled QD structure considered here (see sketch in Fig. 2), zero field single-particle orbitals consist of symmetric (S) and antisymmetric (AS) orbitals with cylindrical symmetry due to a 2D harmonic confinement with a characteristic energy $\hbar\omega_0$. A vertical field preserves the symmetry, but splits the energy shells with non-zero angular momentum (p, d, ...) and gives

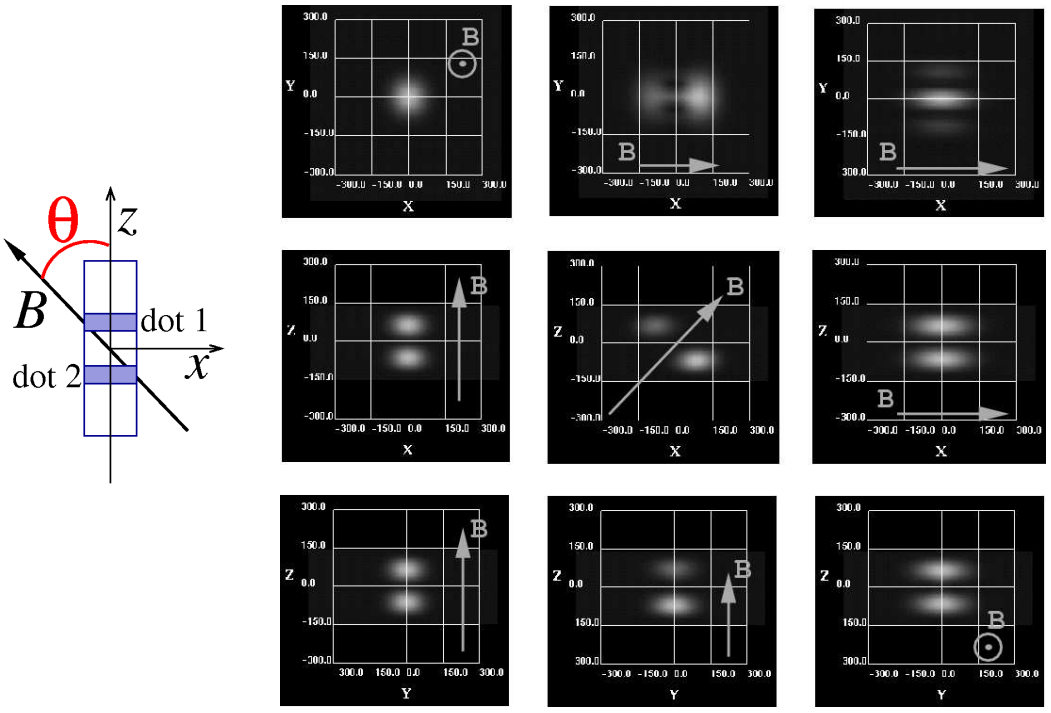

Fig. 2. Single-particle ground state for a GaAs AM. The well width of each dot along the growth direction is 10 nm, the inter-dot potential barrier is 3 nm thick with an offset of 300 meV, and the lateral confinement energy $\hbar\omega_0$ is 10 meV. Lengths are in Å. From left to right column: magnetic field of 30 T at 0°, 45°, and 90° with respect to the growth axis. The geometry and axis definition are sketched on the left.

rise to the well known Fock-Darwin level structure [5] which, in symmetric AMs, is replicated for S/AS levels.

When a finite in-plane component of the field is applied by, e.g., rotating the sample with respect to the field, the energy spectrum (not shown here) may be affected in two ways. First, anticrossing between S and AS levels may occur depending on the angular momentum component. Second, S/AS gaps may be reduced, indicating that tunneling is suppressed by the in-plane field [6].

The effect of an in-plane field on the single-particle wavefunctions is exemplified in Fig. 2 for a typical vertically coupled QD structure. The field is increasingly rotated with respect to the growth axis from vertical (left panels) to horizontal (right panels) plane. In the top row the charge density is shown in the plane perpendicular to the growth axis. When $B_\perp$ is switched on by tilting the total field, the cylindrical symmetry of the system is broken. Angular momentum is not a good quantum number anymore, and energy shells with non-zero angular momentum split and mix as the in-plane field increases. This results in modulations in the charge density, as shown in Fig. 2. In the middle and bottom row the charge density is shown in two planes which contain the growth axis and parallel (middle row) or orthogonal (bottom row) to the field.

It is shown that single particle states are modified in such a way that the lobes of the wavefunctions located in either QD are shifted in the plane identified by the field and the growth direction, if both $B_\perp$ and $B_\parallel$ are non-zero. On the other hand, if only one component of the field is present, the $z \to -z$ symmetry is recovered, and the lobes are vertically aligned. Moreover, comparing the left and right panels one can see that the wavefunctions are squeezed in the direction of the field, as expected. Therefore, a sufficiently large in-plane field suppresses tunneling, and S and AS orbitals become degenerate.

3 Single-triplet transition

We next consider the two-electron system. At low vertical fields the ground state of single and coupled QDs is known to be a singlet state [7,8]. In the moderate field regime, therefore, the lowest energy levels are nearly unaffected by the rotation except for the shift due to the reduction of the tunneling energy, with the singlet state being the lowest.

At sufficiently high vertical field one or more (depending on the sample parameter) singlet-triplet transitions take place at given threshold fields, with the triplet state eventually being the stable one. Since a finite $B_\parallel$ affects the tunneling and, therefore, the exchange energy, the threshold fields will be lowered as $B_\parallel$ increases. This is shown in Fig. 3. The singlet state is stable in the low field regime. The triplet state becomes favored in the large field regime; is should be noted, however, that this happens by different mechanisms whether $B_\perp$ or $B_\parallel$ is large. In the former case, the squeezing of the wavefunction has a Coulomb energy cost which can only be avoided by triplet spin order. This is analogous to single QDs. However, while a finite $B_\parallel$ would not affect very much electronic states in single QDs, where single-particle gaps are large, in AMs the in-plane field affects the S/AS gap; when this vanishes, no tunneling energy is lost by paralleling the electron spins, and the triplet state is favored.

In Fig. 3 we also show in the insets the character of the two-electron wavefunction of the ground state. In the low $B_\parallel$ regime, the two electrons occupy only the S state, either with the s symmetry with opposite spin (low field) or the s and p symmetry levels with the same spin orientation (high field), since a large vertical field reduces the $s - p$ gaps. In the large $B_\parallel$ regime, on the contrary, S and AS states become degenerate, and are equally occupied by the two electrons, due to Coulomb correlations.

Finally, in Fig. 4 we show the exchange energy at zero vertical field. This is positive (i.e., the singlet is the ground state) at low fields, but rapidly decreases as the field increases. At large fields, the exchange energy changes sign, being eventually dominated by Zeeman energy.

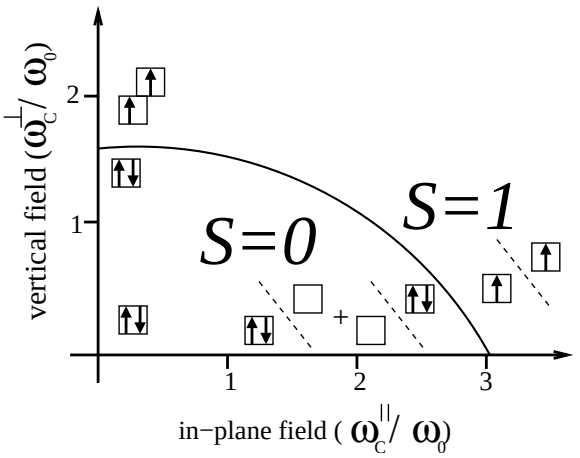

Fig. 3. Single-triplet phase diagram calculated for a GaAs AM made of two QDs 10 nm wide along the growth direction, a 3 nm wide barrier, and lateral confinement energy $\hbar\omega_0 = 4$ meV. The insets show the single-particle occupation in terms of S (left to the dashed lines) and AS orbitals (right to the dashed lines). At low $B_{||}$ only S orbitals are occupied. B is expressed in terms of the cyclotron frequency $\omega_c = eB/cm^*$, m^* being the effective GaAs electron mass.

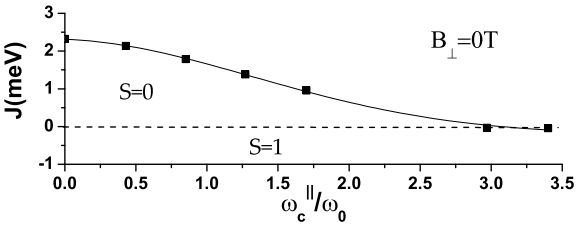

Fig. 4. Exchange energy $J = E_{S=0} - E_{S=1}$ for a a GaAs AM. Same parameters as in Fig. 3.

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References

[1] M. Rontani, F. Troiani, U. Hohenester, E. Molinari, Solid State Commun. 119 (2001) 309–321, special Issue on Spin Effects in Mesoscopic Systems.

[2] M. Pi, A. Emperador, M. Barranco, F. Garcias, K. Muraki, S. Tarucha, D. G.

Austing, Phys. Rev. Lett. 87 (2001) 066801.

[3] G. Burkard, G. Seelig, D. Loss, Phys. Rev. B 62 (2000) 2581.

[4] M. Rontani, G. Goldoni, F. Manghi, E. Molinari, Europhys. Lett. 58 (2002) 555.

[5] L. Jacak, P. Hawrylak, A. Wójs, Quantum dots, Springer, Berlin, 1998.

[6] Y. Tokura, S. Sasaki, D. G. Austing, S. Tarucha, Physica E 6 (2000) 676–679.

[7] U. Merkt, J. Huser, M. Wagner, Phys. Rev. B 43 (1991) 7320.

[8] J. H. Oh, K. J. Chang, G. Ihm, S. J. Lee, Phys. Rev. B 53 (1996) R13264.